ACCURACY OF DIFFERENTIAL SENSITIVITY FOR ONE-DIMENSIONAL SHOCK PROBLEMS

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The technique called Differential Sensitivity has been applied to the system of Eulerian continuum mechanics equations solved by a hydrocode. Differential Sensitivity uses forward and adjoint techniques to obtain output response sensitivity to input parameters. Previous papers have described application of the technique to two-dimensional, multi-component problems. Inaccuracies in the adjoint solutions have prompted us to examine our numerical techniques in more detail. Here we examine one-dimensional, one material shock problems. Solution accuracy is assessed by comparison to sensitivities obtained by automatic differentiation and a code-based adjoint differentiation technique.

INTRODUCTION

Expert use of a hydrocode for design or design-optimization purposes requires information about how some result (or response, R) will change when some code parameter (α) is changed. One can always start by changing parameters one at a time and form a finite difference sensitivity. This method, which we call the Direct Method, requires n+1 computer runs to determine sensitivities to n problem parameters.

A sensitivity technique (1-3) used successfully in the early eighties (4-6), which is called Differential Sensitivity Theory (DST) when addressing the differential equations and Differential Sensitivity Analysis (DSA) when addressing the finite-difference equations, is applied in this effort to a system of time-dependent continuum mechanics equations. Differential sensitivity can be used either in the forward or adjoint mode to determine exact sensitivity derivatives, i.e., if a calculational result or response of interest is R_j and α_i is an input parameter, then (dropping the subscripts) $\partial R/\partial\alpha$ is the sensitivity.

DSA and DST both address the differentiated physical equations (i.e., physical equations differentiated with respect to a parameter α) that are subsequently solved numerically by some code. DSA solves the difference equations (a set of algebraic equations), whereas DST numerically solves the differential equations (a set of partial differential equations, PDEs) and, in principle, is not tied to any particular choice of hydrocode or numerical scheme. In the adjoint mode, DST and DSA obtain the sensitivities to all of the problem parameters in only two computer runs.

Automatic Differentiation (AD) and the Adjoint Differentiation In Code Technique (ADICT) (7), other methods applied to this problem, address the numerical code itself. AD programs take as input the original code and analyze it line by line, providing a code that can produce the needed derivatives. AD programs utilized here include GRESS (GRadient Enhanced Software System) (8) and ADIFOR (Automatic DIfferentiation of FORtran) (9). The ADICT method is similar in concept to AD when utilized in the adjoint mode, but the implementation of the idea varies. Whereas AD operates on a line by line basis, the ADICT method advocates grouping together code in subroutines whenever possible, and each subroutine is analyzed individually. This results in fewer global gradient variables to store and is often more efficient than AD-generated code. Individual derivative expressions produced by AD-generated code, however, are often useful in the

implementation of the ADICT method. Of the AD programs, ADIFOR can only operate in the forward mode, while GRESS can operate in both forward and adjoint modes. Here, ADICT is applied only in the adjoint mode.

In previous works (10-12) we have described the derivation and solution of DST adjoint sensitivity equations for the purpose of computing sensitivities for high-rate, 2D, multi-component, high-deformation problems that contain material strength. Here, we begin with a description of the various sensitivity methods available. Three methods: Forward DSA (FDSA), Adjoint DSA (ADSA), and Adjoint DST (ADST) will be briefly described, and then applied to a simple 1D metal flow problem to investigate the equivalence and numerical accuracy of the methods.

PHYSICAL EQUATIONS

The physical system of equations is the set of 1D Eulerian conservation equations for mass, momentum, and internal energy and an equation-of-state (EOS) augmented with an expression for artificial dissipation. As an example, we follow the development of the momentum equation for the various tecniques:

$$\rho\left[\frac{\partial u_z}{\partial t}+u_z\frac{\partial u_z}{\partial z}\right]=-\frac{\partial P'}{\partial z} \qquad (1)$$

In this equation the dependent variables are density ρ, velocity u_z, and the pressure P' (the sum of an EOS pressure (a function of ρ and internal energy i) and a scalar artificial dissipation).

The finite difference form of Eq. 1 used in this effort assumes an explicit solution, staggered spatial grid, and upwind/donor differences for the convective derivative terms:

$$\rho^n_{j+1/2}\ \mathrm{CD}(u_z)^{n+1}_{j+1/2}=-\mathrm{GRAD}(P')^n_{j+1/2} \qquad (2a)$$

where the finite-difference operators CD, GRAD and DIV are defined using the arbitrary scalar s, vector v and scalar/vector q with the indices n and j designating the time and spatial grids, respectively:

$$\mathrm{GRAD}(s)^n_{j+1/2}\equiv\frac{s^n_{j+1}-s^n_j}{\Delta z} \qquad (2b)$$

$$\mathrm{CD}(q)^{n+1}_j\equiv\frac{q^{n+1}_j-q^n_j}{\Delta t}+u^n_{z,j}\,\mathrm{DONOR}(q)^n_j \qquad (2c)$$

$$\mathrm{DIV}(v)^n_j\equiv\frac{v^n_{j+1/2}-v^n_{j-1/2}}{\Delta z} \qquad (2d)$$

$$\mathrm{DONOR}(q)^n_j=\frac{q^n_j-q^n_{j-1}}{\Delta z},\quad \text{for } u_z>0 \qquad (2e)$$

DSA EQUATIONS

The finite difference form of the physical equation given by Eq. 2a is next differentiated with respect to α giving the DSA forward equation set in terms of differentiated dependent variables,

$$\bar{y}=\left(\left(\frac{\partial\rho}{\partial\alpha}\right)^n_j,\left(\frac{\partial u_z}{\partial\alpha}\right)^n_{j+\frac12},\left(\frac{\partial i}{\partial\alpha}\right)^n_j,\left(\frac{\partial P'}{\partial\alpha}\right)^n_j\right)^T \qquad (3a)$$
$$\equiv\left(\Psi^n_j,\Phi^n_{z,j+\frac12},\Gamma^n_j,\Pi^n_j\right)^T$$

to obtain:

$$\Psi^n_{j+\frac12}\,\mathrm{CD}(u_z)^{n+1}_{j+\frac12}+\rho^n_{j+\frac12}\times$$
$$\left[\mathrm{CD}(\Phi_z)^{n+1}_{j+\frac12}+\Phi^n_{z,j+\frac12}\,\frac{u^n_{z,j+\frac12}-u^n_{z,j-\frac12}}{\Delta z}\right] \qquad (3b)$$
$$+\mathrm{GRAD}(\Pi)^n_{j+\frac12}=0$$

The system of linear algebraic equations represented by Eq. 3b can be rearranged into matrix form as

$$\bar{y}^{n+1}=\underline{A}\,\bar{y}^n+\bar{s} \qquad (4)$$

where $\bar{y}$ is the dependent variable vector given by Eq. 3a. With this matrix form, the DSA adjoint equation set can be obtained by transposing in space and time to give

$$\bar{y}^{*n}=\underline{A}^T\,\bar{y}^{*n+1}+\bar{s}^* \qquad (5)$$

The forward equations given by Eq. 4 can be easily solved for the sensitivities given by Eq. 3a with an

appropriate source $\bar{s}$ specified for a single parameter of interest. Alternatively, the adjoint or transposed equations given by Eq. 5 can be solved for an adjoint solution with an appropriate source $\bar{s}^*$ specified for a single response of interest; this adjoint solution is then combined with the physical solution in various integrals to obtain the sensitivities to all the parameters (10-12).

ADJOINT DST EQUATIONS

Deriving the DST adjoint for Eq. 1 was presented in Refs. 10 and 11 giving the following equation in 3D:

$$-\rho\nabla\Psi^* - \rho\left[\frac{\partial\bar{\Phi}^*}{\partial t} + (\vec{u}\bullet\nabla)\bar{\Phi}^*\right] + \rho(\nabla\vec{u})\bullet\bar{\Phi}^* \\ -\nabla\left(\frac{\partial P'}{\partial i} I^*\right) + \rho\nabla i\, I^* + \nabla\left(\frac{\partial P'}{\partial(\nabla\bullet\vec{u})}\Pi^*\right) = s_\Phi^* \tag{6}$$

where the gradient, divergence and dyad operators appearing in Eqs. 6 are taken to be 1D for the purposes of this effort. The dependent variables appearing in Eq. 6 (with SI units given in parentheses, [R] indicating units of the response) are the adjoint density Ψ^* ([R]/kg), the adjoint velocity Φ_z^* ([R]/N-s), the adjoint energy I^* ([R]/J) and the adjoint pressure Π^* ([R]/Pa-m^3-s). The definition of the adjoint source $\bar{s}^*$ depends on the desired response, and is discussed in more detail in Refs. 10 and 11.

ADJOINT DST DIFFERENCE OPERATORS

In order to numerically solve the DST adjoint equations an appropriate choice for finite difference approximations for the differential operators (divergence, gradient, etc.) must be selected. One choice might be to prescribe ad hoc difference operators, taking care to correctly propagate the adjoint boundary conditions and initial conditions into the solution domain. Previous efforts (10-12) utilized this approach, realizing reasonable but not highly accurate sensitivity results using a donor-cell, staggered-mesh scheme much like the scheme used for solution of the physical equations. A better approach is to use the method-of-support or compatible operators advocated by Shashkov (13) that utilizes inner product properties for continuous functions. This methodology can be used to derive difference operators for the DST equations that are compatible to the difference operators used in the solution of the physical equation set. Although discussed in detail in Ref. 13 an example is given here that finds the difference operator for $\rho\nabla\Psi^*$ appearing in Eq. 6. This example uses the integral identity (i.e., integration-by-parts) for the gradient operator that when specialized to our purpose of finding the difference operator for away from domain boundaries gives the result

$$\int_V \rho\,\Psi^*\left(\nabla\bullet\bar{\Phi}\right)dV = -\int_V \rho\,\bar{\Phi}\bullet\nabla\Psi^*\,dV \\ -\int_V \Psi^*\,\bar{\Phi}\bullet\nabla\rho\,dV \tag{7}$$

Now identifying as prime operators (13) the original DIV and DONOR difference operators defined by Eqs. 2d and 2e for the physical equations, and substituting these into Eq. 7 gives the finite difference form:

$$\sum_j \rho_j\,\Psi_j^*\,\mathrm{DIV}(\Phi_z)_j\,\Delta z = -\sum_j \Phi_{z,j}\,\rho\nabla\Psi^*\Delta z \\ -\sum_j \Psi_j^*\,\Phi_{z,j}\,\mathrm{DONOR}(\rho)_j\,\Delta z \tag{8}$$

Expanding the summations, substituting in the DIV and DONOR definitions, and solving for the unknown gradient operator $\rho\nabla\Psi^*$ gives the compatible finite difference approximation (for $u_z > 0$):

$$\left(\rho\nabla\Psi^*\right)_{j+\frac{1}{2}} = \frac{\rho_{j+1}\Psi_{j+1}^* - \rho_j\Psi_j^*}{\Delta z} \\ -\frac{1}{2}\left[\Psi_j^*\,\frac{\rho_j - \rho_{j-1}}{\Delta z} + \Psi_{j+1}^*\,\frac{\rho_{j+1} - \rho_j}{\Delta z}\right] \tag{9}$$

Note that the spatial grid point for $\rho\nabla\Psi^*$ is located at the cell edge $j+1/2$, appropriate for use in the cell-edged adjoint momentum equation. This procedure can be repeated using various integral identities to define all the difference operators in

Eq. 6, forcing all these operator definitions to be compatible with the physical equation operators given by Eq. 2b-e. *Comparison of these derived DST compatible operators to the implied spatial operators appearing in the adjointed (transposed) DSA equations represented by Eq. 5 shows the two difference operator sets to be identical, and therefore the two methods should produce identical numerical results.*

METAL FLOW TEST RESULTS AND DISCUSSION

Consider the 1D flow of a metal plate which has an initial velocity of 500 m/s, an initial density of 8000 kg/m^3, and a sound speed of 4000 m/s. The plate is 2 mm in thickness and is divided into ten 0.2 mm cells for the numerical computations. At the initial time the right side of the plate instantaneously decelerates to 400 m/s. This produces a left-going shock that compresses the material to a Hugoniot pressure of 21 GPa. Numerical solution was performed using the boundary and initial conditions given above to a final time of 1.0 μs. Sensitivities for representative problem parameters using the six different sensitivity methods discussed above were then generated, and the results are given in Table 1 for a space/time averaged pressure response. The parameters as listed in the table are initial density, initial velocity, and the EOS sound speed. ADIFOR, ADICT and FDSA all show excellent agreement for 5, 6 or more digits. The direct method sensitivities were only converged to 3 or 4 digits. For our purposes the AD results can be considered exact. The two adjoint techniques, i.e., DSA adjoint and DST adjoint, also all show excellent agreement for 5, 6 or more digits. However comparison of the forward results with the adjoint results reveal agreement to only 3 to 4 digits; *in principle all the methods should agree*.

We speculate that this lack of consistency between the forward and adjoint DSA/DST results becomes more severe for stronger shock problems containing additional complexity in terms of constitutive modeling, multi-material discontinuities and increased dimensionality, thus explaining the inaccuracy observed in our previous work.

Table 1. Sensitivity Comparisons for an Average Pressure Response

	Sensitivity		
Method	**Initial Density**	**Initial Velocity**	**Sound Speed**
Direct	$1.594500 \cdot 10^7$	146500.0	154080.0
ADIFOR	$1.592504 \cdot 10^7$	146255.7	153885.7
ADICT	$1.592504 \cdot 10^7$	146258.3	153885.6
FDSA	$1.592504 \cdot 10^7$	146254.3	153888.0
ADSA	$1.592504 \cdot 10^7$	145760.2	153870.5
ADST	$1.592504 \cdot 10^7$	145766.0	153870.4

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